JPLS CDR report

Review committee: M. Fukuto, M. Zhernenkov, S. Coburn, L. Stiegler, R. Farnsworth, L. Wiegart (chair)

Reviewed material:

- Presentation by B. Ocko
- Presentation by D. Babescu
- Slides about cost/schedule and excel budget sheet supplied by C. Stebbins

Description of the project and conceptual design

The JPLS project is aimed at 'jump starting' the PLS beamline, an eventual canted buildout of 12ID. The conceptual design of 12ID included two endstations: one that was realized as SMI and a liquid surface scattering endstation to be hosted in a separate hutch. The latter was envisioned to start operation in time-shared mode with SMI, but with the potential to become an independent canted branch of 12ID. This liquid surface scattering endstation was eventually removed from the scope of the NEXT project under which 12ID was build, except for some infrastructure (endstation hutch, utilities, etc.). A new endstation for Polymer processing and liquid surface scattering (PLS) was proposed, but failed to secure sufficient funding for a canted buildout. With the return of the liquid spectrometer from APS and the instrumentation available from the X22B beamline at NSLS, it was decided to give the PLS beamline a head start by building an endstation to be operated in time-shared mode with SMI, using the existing ID and optics. The endstation is mostly to be built with re-used equipment on a 1.5M$ (materials and labor) budget and an 18 month schedule.

The target capabilities for this endstation were stated as a world class instrument for:

- Polymer processing in environments approaching those in industrial settings
- Liquid interfaces: static self-assembly and dynamics of evaporation
- XRR, GI-fluorescence, GISAXS, GIXD
- Liquid sample cells, such as Langmuir troughs
- Processing sample environments, such as roll-to-roll, Vapor Phase Deposition chambers,..
- 5 micron beam size, 8-24 keV energy range, high x-ray flux for sub-second to minute time-resolution

Two conceptual designs were presented:

'A': WAXS and XRR detectors are coupled to the sample stage, while the SAXS detector is located on a separate positioning platform ~3m downstream of the sample. The design would be somewhat compatible to SAXS experiments using large sample environments that are not located on the sample stage. A solution for an evacuated flightpath for SAXS was not available at this time.

'B': All three detectors (XRR, WAXS, SAXS) are coupled to the sample stage and each other. The SAXS detector would end up at a relatively short sample detector distance of 1.5m (possibility to increase this to 2m was mentioned during the review).

Both designs re-use an existing single crystal deflector for beam steering, as well as a CCD as SAXS detector and a Pilatus 100k as the detector for X-ray reflectivity.

Findings

- Design ‘A’ provides more open space that could enable unique research capabilities, e.g polymer processing with ‘real world’ instrumentation to be brought into the hutch. The sample-detector distance for the SAXS detector is ~3m. This design is currently lacking a concept for the SAXS flightpath.
- Design ‘B’ is more complete, e.g. including a solution for a SAXS flightpath, but has other challenges, e.g. no open space to roll in large sample environments, the coupled in-plane rotation of all detectors or the relatively short (1.5-2m) sample-detector distance for SAXS.
- For either of the two designs, it is unclear how much of the newly built equipment could be re-used in a canted build-out.
- The decision about which design path to continue has not been made. Decision making is hampered by conflicting boundary conditions and scope, such as time-line, budget, instrumentation available and target capabilities.
- Either design would provide a sample space that is larger than those available at related NSLS-II beamlines (e.g. SMI and CMS), however, whether the designs are useful for ‘real-world’ polymer processing is unclear. Currently there is no involvement of academic or industrial partners for this research area.
- Neither design A or B follows the design developed for PLS (independent sample and detector positioning, providing more flexibility for large sample environments)

Recommendations

- Clarify/prioritize the scope of work as soon as possible. The existing designs seem to focus very much on liquid surface scattering and might miss some opportunity for unique capabilities in polymer processing, that are not only part of the stated scope, but might also be the most promising route to secure funding for an eventual canted buildout. Not all stated capabilities will be within reach for JPLS (e.g. excellent time resolution for matter far out-of-equilibrium).
- In order to guide the decision and refine the design, input from a larger community would be desirable, if it is possible within the tight timeline. A BAT and/or workshop would be ideal, and direct contact and feedback from some selected experts might provide a more timely input.
- Clarify the scope with respect to whether or not investments made in JPLS should be re-usable for a future buildout. This concerns including e.g. encoders and additional motorized adjustments into the design, even though it might not be implemented within the scope of JPLS, but provide a simple and cost effective route to upgrade instrumentation later. This also concerns travel ranges of newly designed stages, etc. Consider keeping the long translations compatible with a level floor that would be essential for large roll-in equipment (e.g. use flat marble ‘tiles’ or simply polished concrete floor for the air-pads, instead of bulky granite slabs that might turn out to be in the way down the road).

Technical Risks

Finding: The JPLS project re-uses substantial amounts of endstation (mostly positioning) equipment from the APS and X22B spectrometers, parts that are ~20 years old. For a subset of positioners, e.g. the Eulerian cradle (Huber 511) for the single crystal deflector, the accuracy requirements are tight or even exceeding the original specifications. The status/performance of these components has not yet been checked/tested.

Recommendation: Verify as soon as possible the performance of key components. Develop in parallel backup plans, such as sending components back to the manufacturer for measurements/refurbishment, equipping stages with encoders, get quotes/lead times for new components. Besides the necessity to achieve a performance that would make the endstation work, re-usability of new/upgraded equipment in a future buildout might guide the decision (e.g. can the Eulerian cradle be re-used for a double deflector stage? Will the canted buildout still use a single crystal deflector to increase beam separation, as in the CDR for 12ID?).

Finding: Design 'B' couples all three detectors and the SAXS beamstop to the same in-plane rotation and to the center of the sample stage.

Recommendation: Consider adding some flexibility to move detectors relative to each other and a more flexibility between sample stage and detectors stage (as in the PLS design).

Finding: It was mentioned that some focusing at the endstation instrument would be highly desirable, in particular for scattering from liquid interfaces. Assuming budgetary constraints, no attempt has been made so far to include focusing in the design.

Recommendation: Providing a solution for full energy tuneability will likely be too much for the scope of the project. However, providing focusing at a single energy, e.g. with a stack of CRLs, might be the most cost-effective option to achieve some state-of-the-art capability and should be evaluated for 'day 1' implementation or later upgrade.

Scientific Risks

Finding: Due to spatial constraints inside the existing hutch, the sample-detector distance for (GI)-SAXS is rather short (~3m in design 'A', 1.5-2m in design 'B'). Design 'B' in particular only allows for an unusually short distance. It was pointed out that some SAXS experiments were carried out at 1.5m during the technical commissioning of the CHX beamline (using an Eiger1M), however, at about 1/3rd of the 24keV max energy targeted for JPLS. Estimates of the required resolution based on the scientific scope are not yet available.

Recommendation: Check the science case for resolution requirements for SAXS, particular at higher energies and in case a very short sample-detector distance of ~1.5m is pursued.

Finding: Roughly half of the non-labor budget (46%) is foreseen for the purchase of a Pilatus 1M, used for fast (non-scanning) GIXD. While it will certainly work for its –limited- intended use, it is not clear whether this would be the most sensible investment. It would enable very fast (CHX demonstrated 30ms GIXD from a monolayer at the liquid-air interface @150mA) GIXD, while reflectivity (because of the use of a single crystal deflector) and GI(SAXS) (slow CCD) would have poor time resolution. In particular the use of a slow CCD for (GI)SAXS would be sub-standard for ID beamlines at 3rd generation storage rings. More importantly, it is unclear how the Pilatus 1M would be used in the future buildout of (J)PLS: for polymer processing, a tiled WAXS detector (with an aperture for the SAXS signal) is almost indispensable, as the WAXS signal can be expected to be anisotropic. Re-purposing the Pilatus 1M at that time as a SAXS detector would severely limit the q-resolution, due to the short sample-detector distances achievable in the existing hutch and the large pixel size of the detector.

Recommendation: Look into alternatives for the Pilatus1M, considering future requirements and availability of other detectors (including CCD for WAXS, Eiger1M in the equipment pool,…).

Safety Aspects

There are no additional safety concerns related to installation and operation of the JPLS concept. The items to consider are:

- Ensuring re-used equipment is in accordance with current NSLS-II requirements (i.e. electrical)
- A snorkel exhaust will be the minimum exhaust required for these experiments. Airborne monitoring may show that experiment enclosure will need to be considered.
- A plan needs to be developed for the storage/movement of the SMI beam pipe when JPLS is in use
- The design needs to ensure that the JPLS equipment can be moved out of the way for the SMI beam pipe installation, and that personnel will have adequate clearance around the granite table to avoid ergonomic challenges.
- Check whether the shielding of the hutch downstream wall is sufficient to stop the steered beam or if additional shielding (like the beamstop in other hutches) is required.

Budget / Schedule

Finding: The current schedule shows a PDR date of Dec 21st 2017. A large number of procurements are scheduled for Dec 22nd 2017, well before the FDR (May 2nd 2018). Procurement of endstation hardware (which includes machined parts) only starts 2 weeks before start of assembly, controls design and development is completed one week after the CDR, etc. The mechanical designs presented at the CDR were very detailed, which gives confidence that rapid progress can be made once the conceptual design is locked-in.

Recommendation:

- the schedule is tight and the date for the PDR appears to be unrealistic at this time; should be shifted to a later date

- include a plan to test equipment that will be re-used from APS/NSLS and a plan to refurbish/replace components as necessary
- allow for some time between PDR and procurement of custom components, such as slides, ballscrews and granites
- if the schedule is intended to be used for resource loading and planning, make sure that the dependencies of the individual activities are properly captured
- controls and computational complexity might not be fully understood at this point, keep controls group involved as the design progresses to allow for resource planning

Finding: some items in the budget seem low (machined parts, encoders) and there is no 'miscellaneous' budget item which would take into account that not all costs can be correctly estimated at this early stage. On the other hand, some costs seems to be high, such as a total of ~80k$ for beam visualization (including cameras) and beam monitors.

Recommendation:

- if there is no other source of contingency, consider purchasing the 'nice to have, but not essential' items later than currently envisioned in the schedule, after some risks, such as performance of old equipment and uncertainties about the design, are retired. Such items are: fluorescence detector [available in the equipment pool; with 30% of user time for JPLS and assuming 50% of GUPs needs this detector ->~6 weeks/year]; controls station furniture and partitions [can share space with SMI to start]
- beam stabilization at the SSA is provided by SMI, any feedback on endstation positioners (stepper motors) will be slow and can be realized in EPICS: P. Ilinski recently reviewed beam monitoring/feedback options for the BST, including in-house electronics and resistive diamond XBPMs which might be significantly cheaper than the budgeted 30k$. Check available designs for beam visualization.

Miscellaneous

- (GI)SAXS experiments will need an aperture closer to the sample to clean up the beam after the beam defining slits.
- Expected performance of the beamline in term of the X-ray beam (e.g. flux vs. energy vs. beamsize) was excluded from the review by the JPLS team.